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SOME TECHNICAL CONSIDERATIONS IN MULTIDIMENSIONAL SCALING

by ROBERT F. BOLDT

Statistical Research and Analysis Laboratory

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**SOME TECHNICAL CONSIDERATIONS IN
MULTIDIMENSIONAL SCALING**

By Robert F. Boldt

STATISTICAL RESEARCH AND ANALYSIS LABORATORY

Cecil D. Johnson, Chief

U. S. ARMY PERSONNEL RESEARCH OFFICE

**Office, Chief Research and Development
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FOREWORD

A portion of the research effort of individual U. S. APRO research scientists is devoted to basic research designed to extend the capability of human factors research in terms of knowledge, techniques, and methodology which can ultimately be applied in seeking solutions to Army operational problems. This in-house laboratory independent research is conducted under the Department of Army Research and Development Project No. 2T013001A708, FY 1965 Work Program.

The present Technical Research Note reports on a study conducted within the Statistical Research and Analysis Laboratory. The study as originally conceived dealt with a methodology developed for multidimensional scaling in the definition and measurement of human values. While the scaling problem was not carried to completion because the data were found to be inadequate for the statistical model, the very difficulties encountered led to certain methodological advances which could facilitate further development in application of the method.


J. E. UHLAUER
Director of Laboratories

SOME TECHNICAL CONSIDERATIONS IN MULTIDIMENSIONAL SCALING

BRIEF

In an examination of problems arising in multidimensional scaling, the multivariate analysis of interpoint distances into coordinates in m -dimensional Euclidean space is first described. Problems encountered in application of the method are then presented, and solutions developed or suggested by the writer are discussed.

The first difficulty was the occurrence of a complex additive constant during the course of Messick-Abelson iterations for solutions of relatively low dimensionality. A regression approach is suggested as a reasonable alternative. This approach cannot yield a complex additive constant and has been successfully used where the more common method has failed.

A second problem arose because the common Hotelling method of extracting characteristic roots and vectors does not find the vectors in the algebraic order of the roots. This difficulty, combined with the relative slowness of the Hotelling method, recommends the use of Jacobi's method.

A third problem was the occurrence of negative "distances" obtained when the final additive constant is added to the scale values. It was conjectured that this result may arise in samples even when a proper dimensionality has been defined and the solution sought. A model sampling study of a one-dimensional system supported the conjecture. Hence, the occurrence of such negative "distances" is not necessarily indicative of an underlying structure of higher dimensionality.

Finally, it was pointed out that the occurrence of negative "distances" is actually built into the successive intervals and comparisons approaches. Alternative assumptions were discussed.

SOME TECHNICAL CONSIDERATIONS IN MULTIDIMENSIONAL SCALING

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SOME TECHNICAL CONSIDERATIONS IN MULTIDIMENSIONAL SCALING

INTRODUCTION

Papers by Young and Householder (1) and Richardson (2) and later by Torgerson (3) and Messick and Abelson (4) mark the development of a methodology for representing the organization of persons' perceptions of classes of stimuli as a configuration of points in psychological space. The methods used rely on estimating as numbers the perceived differences among all pairs of a group of stimuli. Numbers representing differences of stimulus pairs are interpreted as distances among points. If the model is appropriate, the distances are considered Euclidean. Coordinates on a set of basic dimensions can then be found. These techniques have been used to analyze judgments on a wide variety of stimuli. Most such applications are not of an applied nature, although a more recent report by Siegel and Smith (5) describes an application of the method to a problem in job analysis. Because of the rapidly growing body of studies using the method and the anticipated expansion of practical applications, it is appropriate to describe certain problems that have been encountered in the use of the technique and to provide such solutions as have been obtained. Prior to this description it will be useful to describe the multivariate analysis utilized to translate interpoint distances into coordinates in m-dimensional Euclidean space.

DISTANCES INTO COORDINATES

As mentioned above, a key step of the multidimensional scaling procedure is to resolve interpoint distances into coordinates. If d_{ij} is the distance between stimuli i and j which are located in m -dimensional psychological space, then

$$d_{ij} = \sqrt{\sum_{k=1}^m (a_{ik} - a_{jk})^2} \quad (1)$$

where the a_{ik} is the coordinate of the i th point in the k th dimension. Squaring both sides of (1) and expanding the expression in parentheses on the right-hand side, obtain

$$d_{ij}^2 = \sum_{k=1}^m a_{ik}^2 + \sum_{k=1}^m a_{jk}^2 - 2 \sum_{k=1}^m a_{ik} a_{jk} \quad (2)$$

There would be $\frac{n(n-1)}{2}$ such equations where n is the number of stimuli.

The following matrices are defined:

D is an $n \times n$ matrix with elements d_{ij}^2 .

L is an $n \times 1$ column of 1's.

A is an $n \times 1$ column with entries $\sum_{k=1}^m a_{ik}^2$.

\tilde{F} is an $n \times m$ matrix of coordinates.

I is the $n \times n$ identity matrix.

$W = (I - (1/n) L L')$.

Then the equations (2) in matrix form are

$$D = A L' + L A' - 2 \tilde{F} \tilde{F}'. \quad (3)$$

Premultiplying and postmultiplying both sides of (3) by W, noting that $WL = 0$, yields

$$W D W = - 2 W \tilde{F} \tilde{F}' W. \quad (4)$$

When the matrix operations involved in $W \tilde{F}$ are traced, the result is seen as the subtraction of a constant from each column of \tilde{F} , so that the sum of each column is zero (the constant will usually be different for each column). Geometrically, this subtraction has the effect of placing the origin of the space at the centroid of the points and has no effect on the interstimulus distances. We therefore define $F = W \tilde{F}$ and modify equation (4) to

$$F F' = - (1/2) W D W. \quad (4a)$$

Then, if D is known, a usual factorial decomposition of the right-hand side of (4a) will yield the coordinates within an arbitrary centering and orthogonal rotation. Unfortunately, with the exception of methods used by Helme (6), or empirical methods (7), the elements of D are not known because of the indeterminacy of an additive constant (4) which is due to the nature of the way in which scale values of differences are obtained (8). Both the method of successive intervals and the method of complete triads (3) yield interpoint distances only up to a linear transformation. Neglecting any multiplicative indeterminacy, if s_{ij}

is the scale value associated with the dissimilarity of the i th and j th stimuli, then the additive indeterminacy c can be expressed by relating the d 's and s 's as follows.

$$d_{ij} = s_{ij} + \delta_{ij} c. \quad (5)$$

Where $\delta_{ij} = 0, i = j$

and $\delta_{ij} = 1, i \neq j$

$$s_{ij} = 0, i = j$$

Squaring both sides of equation (5), one can obtain in matrix form

$$D = B + c E + c^2(L L' - I), \quad (6)$$

where B is an $n \times n$ matrix with entries equal to s_{ij}^2 , and E is an $n \times n$ matrix with entries equal to s_{ij} . Substituting the right-hand side of (6) for D in equation (4a) yields

$$F F' = -(1/2)(WBW + cWEW - c^2W). \quad (7)$$

The unknowns in equation (7) are the entries in F and the constant c . Computing experience indicates that the characteristic vectors of the right-hand side of (7) are relatively insensitive to the choice of value of c . Hence one could guess a value of c and then extract the first m factors of the matrix indicated by the right-hand side of (7). For example, suppose X_k is the k th such characteristic vector and M is the matrix obtained from (7) using a particular value for c . Then $X_k' M X_k$ would yield the associated characteristic root. One could take advantage of the relative invariance of the characteristic vectors with change in c , once having found the first m X 's for a particular value of c , by estimating the sum of characteristic roots as a quadratic function with c as an argument, i.e., if $R(c)$ is the sum of characteristic roots, then

$$R(c) = \left(-\frac{1}{2}\right) \left[\sum_{k=1}^m X_k' WBW X_k + c \sum_{k=1}^m X_k' WEW X_k - mc^2 \right]. \quad (8)$$

Similarly, if $S(c)$ is the sum of the diagonals of the right-hand side of equation (7) with c as an argument, then

$$S(c) = -(1/2)((1/n^2)b_{..} - (1/n)b_{.1} - (1/n)b_{.j} + c((1/n^2)e_{..} - (1/n)e_{.1} - (1/n)e_{.j}) - (n-1)c^2). \quad (9)$$

Where $b_{.1}$ and $e_{.1}$ are the diagonals of B and E respectively. To find c , Messick and Abelson (4) equate $R(c)$ and $S(c)$ and solve the resulting quadratic equation for a new value of c which is then used to compute a new M which is used to get new X 's, etc. This procedure, in effect, sets the sum of the $n - m$ remaining roots of M equal to zero. If these roots are small, then the lower rank approximation of M by FF' will be good.

COMPLEX ADDITIVE CONSTANT

The Messick-Abelson additive constant procedure is an ingenious one by which many scaling problems have been solved. However, in several studies, the author has observed procedural difficulties which need to be resolved. These difficulties seem to arise when the chosen dimensionality is small relative to the number of stimuli used. To choose a dimensionality, the investigator guesses some value for c , computes the right-hand side of (7), factors the resulting matrix, and examines the profile of characteristic roots. Where there seems to be a sharp break in the size of the roots, he sets a trial dimensionality and begins additive constant iterations as described above. For example, Boldt (9) followed this procedure on a 15-stimulus problem and found one very large root, the remaining roots being relatively small. However, when single factor iterations were initiated, they could not be completed because of the complex roots of the quadratic equation obtained when $R(c)$ was equated to $S(c)$. Since the analytical procedure as currently designed depends entirely on real numbers, there was no way to proceed. To solve this problem, additional dimensions were added, although the additional dimensions in no way added to the substantive understanding of the study. Complex constants were also encountered by Wiskoff (10) and Olans (11).

To bypass this problem, a procedure is needed for estimating the additive constant which always yields a real number. To find such a method, we first substitute s 's and c for d in equation (1) obtaining

$$s_{1j} + c = \sqrt{\sum_{k=1}^m (a_{1k} - a_{jk})^2} \quad i \neq j. \quad (10)$$

Guessing a value for c , the right-hand side of (7) can be constructed and factored to obtain F for the guessed c and dimensionality. If f_{ik}

is a typical entry in F, then $\sqrt{\sum_{k=1}^m (f_{ik} - f_{jk})^2}$ can be used as a trial estimate of the right-hand side of (10), with the following modification required. Knowing in advance that the constant c will be modified, we can allow for a change in the scale of the distances reconstructed after the next iteration by allowing the estimated distances to be expanded or contracted through multiplication by a constant, q. That is, write

$$s_{ij} + c = \tilde{q} \sqrt{\sum_{k=1}^m (f_{ik} - f_{jk})^2} \quad i \neq j. \quad (11)$$

Since the s's are known and f's are determined using an old c, the constant of regression of s on $\sqrt{\sum (f_{ik} - f_{jk})^2}$ can be found and is equal to minus the new additive constant. This new constant could be used to get new f's and the procedure iterated until the constant ceases to change. When convergence is achieved, the coordinates, a's, are equal to b times the final F.

Clearly, no complex numbers can be involved in this process unless b is negative, i.e., the theoretical distances correlate negatively with the s's. If this happens, it seems reasonable to suspect that something is drastically wrong with the whole conceptualization, provided all computations are right. One way to correct this condition is to reverse the sign of the s's, although it is very difficult to imagine how such a change could be reasonable in the context of multidimensional scaling. No such negative correlation is known to the author.

CHOICE OF FACTORING METHOD

As indicated above, the multidimensional analysis requires guessing a constant, using it to compute the right-hand side of equation (7) and factoring the resulting matrix. Since the regression procedure does not involve calculating characteristic roots, perhaps centroid or square root factoring would be acceptable, although with computers the extraction of characteristic roots and vectors is quite feasible and in fact routine. If characteristic roots and vectors are used, there is some importance in choosing a proper factoring method. Since the number of factors desired is usually less than the order of the matrix to be factored, one would be tempted to use Hotelling iterations (12) which extract one factor at a time. However, this method extracts factors in the order of the absolute value of the characteristic roots. Messick and Abelson (4) have reported some results which render extraction in the order of the absolute value of the roots somewhat less desirable. They have pointed out that not only are the characteristic vectors from (7) relatively insensitive to changes in c, but also that the associated roots remain in the same order, although the magnitude and separation of roots may change as c changes.

Hence, if one makes a sufficiently bad initial guess at the value of c , the matrix to be factored may have strong negative roots. While this problem is not a serious one from the standpoint of numerical analysis, the practitioner should be aware that it can be encountered in practice. If Hotelling iterations (12) are used, these large (in absolute value) negative roots will be extracted. Such roots are incompatible with the distance interpretation of the scale value. Hence the factoring method to be used should extract factors in the algebraic order of the characteristic roots rather than their absolute value. The Jacobi Method (13) is quite adequate in this regard, since it extracts all the factors which can then be selectively chosen in the algebraic order of the roots. This method has also proved to be considerably faster than the Hotelling method.

The difficulty in the order of extracting factors could probably be circumvented if one first did a complete factoring with some guessed value of the additive constant and visually inspected the resulting profile of characteristic roots. However, there is merit to computing routines such that one inputs the scale values, and the computer then works its way to solutions through increasing dimensionality until a satisfactory solution is achieved. The routine currently used by the author uses zero as a guessed constant no matter what the values of the s 's and then uses as a starting constant for higher dimensions the final constant obtained from the solution at the next lowest dimensionality. The inclusion of the Jacobi routine with the factors taken in the algebraic order of the roots has been consistently successful.

To speed up the numerical procedure, an attempt was made to capitalize more fully on the relative invariance of the characteristic vectors with change in c . Suppose the matrices M and \tilde{M} are calculated as indicated on the right-hand side of equation (7) using two different values for c . Then

$$M = P G P'$$

and

$$\tilde{M} = \tilde{P} \tilde{G} \tilde{P}'$$

where P and \tilde{P} are the matrices of characteristic vectors and G and \tilde{G} are diagonal matrices of characteristic roots. The invariance which has been referred to is that

$$\tilde{P} = P + E \quad (12)$$

where the entries in E are small in absolute value. Note that since \tilde{P} is orthogonal, the multiplication $\tilde{P}' \tilde{M} \tilde{P}$ yields a diagonal matrix. It can be expected that the multiplication $P' \tilde{M} P$ would nearly diagonalize \tilde{M} since

$$\begin{aligned} P' \tilde{M} P &= (\tilde{P} - E)' \tilde{M} (\tilde{P} - E) \\ &= \tilde{P}' \tilde{M} \tilde{P} - \tilde{P}' \tilde{M} E' - E' \tilde{M} \tilde{P} + E' \tilde{M} E \\ &= \tilde{G} - (\text{terms in } E). \end{aligned}$$

Since \tilde{G} is diagonal, and since E is small, it would be supposed that the diagonalization of M would be nearly accomplished. Hence use of the old characteristic vectors could be expected to reduce time spent in diagonalizing new M matrices. This conjecture is recorded because at some time it may lead to useful application. However, for the problems on which it was attempted it was found that the Jacobi factoring from scratch was faster, since the required matrix multiplication $P' M P$ was very slow when done in FORTRAN with double subscripts. It is suggested that speed-up could occur if the user of multidimensional scaling had available faster techniques for accomplishing matrix multiplication.

NEGATIVE DISTANCES

Once a solution has been reached, there are two ways of estimating interstimulus distances. One of these is to use the Euclidean distance function (1) and the final coordinates; the other, more commonly used, is to add the constant c to the empirical scale values. The latter method has yielded negative numbers for solutions of relatively low dimensions in the studies of Boldt (9), Wiskoff (10), and Olans (11). Since negative numbers are incompatible with a distance interpretation, solutions at higher dimensions were sought. In the interest of parsimony, however, it is useful to inquire as to what extent these negative "distances" arise as a consequence of sampling fluctuation. To accomplish this inquiry, several successive interval multidimensional scaling samples were simulated using model sampling (14) procedures. Table 1 gives the matrix of interpoint distances used.

Table 1

INTERPOINT DISTANCES MATRIX

Stimulus	Stimulus					
	A	B	C	D	E	F
A	0	0	.5	1	2	4
B	0	0	.5	1	2	4
C	.5	.5	0	.5	1.5	3.5
D	1	1	.5	0	1	3
E	2	2	1.5	1	0	2
F	4	4	3.5	3	2	0

If stimulus A is located at the origin, and entries in the first row of Table 1 are taken as coordinates in a one-dimensional Euclidean space, these coordinates can generate the rest of the table. Hence a one-dimensional system is implied in Table 1. Consistent with the successive interval models (15), the distances were assumed to be normally distributed over presentations. Category boundaries were set at 2,4,6,8, and 10.

Then data for six samples of 20 subjects each were generated and scale values found assuming discriminial dispersions of 20. Multidimensional analysis of the resulting scale values was then accomplished using procedures described above. Only one of the samples gave all positive distances when the additive constant from a one-dimensional solution was added to the scale values. Four of the samples required two dimensions, and the fifth sample would have required five dimensions. The problem was, of course, rigged to produce the result--it was expected that the negative "distance" would occur at the zero distance between stimuli A and B. However, every stimulus pair yielded a negative distance for at least one sample. A majority of the pairs yielded negative "distances" in one or more of the cases where two dimensions were adequate. These results may well be peculiar to the particular configuration of parameters, especially including sample size. The implication is clear, however, that the occurrence of negative "distances" does not necessarily imply a higher dimensionality of the underlying stimulus configurations. Additional research, beyond the scope of the present study, is needed on which reasonable sets of parameters could be used to determine the extent to which these negative "distances" would be due to sampling fluctuation in practical experimentation.

DISTRIBUTION OF INTERPOINT DISTANCES

The results of the model sampling above deal with the case where scale values are obtained by successive intervals techniques and would probably apply to comparisons methods (3). They do not apply to graphic rating procedures. In a personal communication in 1956, Tucker pointed out that both the successive intervals and comparisons methods, as used in practice, assume that stimulus strengths are normally distributed over presentations. In the multidimensional scaling problem, the stimulus strengths are interpreted as interpoint distances. Since the normal distribution has non-zero probability ordinates over the entire real axis, it follows that the occurrence of negative distances is implicit in both the successive intervals and comparisons models. It should not be surprising that negative "distances" occur in some solutions. Assumptions other than normality could be tried. For example, the author (16) has used gamma distribution assumptions to obtain estimates of the distances on a ratio scale, but in that attempt there was no good rationale for the assumption, and the occurrence of complex solutions severely limited the value of the approach. Tucker has pointed out that if, over a large number of presentations, the stimulus points are normally distributed in m -dimensional psychological space, the interpoint distances would take on a non-central chi-square distribution. However, no feasible numerical techniques based on the non-central chi-square are currently available.

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11 SUPPLEMENTARY NOTES	12 SPONSORING MILITARY ACTIVITY OORD	
13 ABSTRACT Three problems encountered in executing the analysis of multidimensional scaling data are presented and their resolutions discussed. The first problem is that complex solutions to a quadratic equation may be encountered during Messick-Abelson additive constant iterations. An alternative iteration sequence is presented which necessarily involves only real solutions. This sequence has been successfully used repeatedly. The second problem is that with a poor initial guess at the additive constant, large negative characteristic roots may occur in matrices which theoretically represent scalar products of coordinates of points located in Euclidean space. A factoring method which simply omits these roots will yield a satisfactory solution. The third problem is that when the final additive constant is added to empirically obtained interpoint distances on a ratio scale, the resulting "distance" is often negative. A model sampling study using successive intervals assumptions demonstrates that such negative "distances" can arise as a consequence of sampling fluctuations, and hence, that the occurrence of such distances is not necessarily indicative of an underestimate of the dimensionality of the configuration of stimulus points.		

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* Multidimensional scaling						
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